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EXPLOSIONS IN VACUUM

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EXPLOSIONS IN VACUUM

Prepared by:
Morton Lutzky

ABSTRACT: The results of an IBM-704 machine calculation of the explosion of a 1-lb. charge of pentolite in vacuum and the expansion of the detonation product gases to strike a concentric rigid spherical target are reported. Alternative equations of state were employed in the calculation (ideal gas with constant γ , and ideal gas with variable γ) and the results compared. Plots are given of pressure and energy density, versus distance, at various times after the wall has been struck, and pressure-time histories of the gas at the wall. Representative values for the peak wall pressure at various distances from the center, for the constant γ case, are 22,712 Bars at 8.0 cms., 805.6 Bars at 24.0 cms., and 5.37 Bars at 128.4 cms. Scaling to other distances and charge weights is considered. A 512-lb pentolite charge, for example, is shown to produce a pressure of 145 psi at the wall some 26 ft away. Such a pressure, if applied to a spacecraft, would probably destroy it.

Approved by:

J. F. Moulton, Jr., Chief
Air-Ground Explosions Division

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EXPLOSIONS RESEARCH DEPARTMENT
U.S. NAVAL ORDNANCE LABORATORY
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Explosions in Vacuum

The problem of explosions in rarefied atmospheres can be attacked by numerical methods using high-speed electronic computers. This report describes a preliminary calculation in which a spherical charge detonates in vacuum, causing the resultant detonation gases to expand and strike a rigid, spherical target. The work was done under NOL Task RUME-3-E-000/212-1/FO08-10-004 (PA 014), and is a partial solution of KEY PROBLEM No. 15, Chapter 7, NAVORD Report 3906, (Key Problems in Explosives Research and Development).

W. D. COLEMAN
Captain, USN
Commander

C. J. Aronson
C. J. ARONSON
By direction

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INTRODUCTION

1. In carrying out a program of investigating the characteristics of blast in a rarefied atmosphere, it is useful to have available a description of the limiting case of zero density in the medium surrounding the charge; that is, an explosion in vacuum. In this case, the explosion consists only of the rapidly expanding detonation products, and the loading produced upon a target is the result only of the impacting detonation gases, without the usual atmospheric blast wave. Numerical calculations have been carried out at NOL on the IBM-704 digital computer to determine the characteristics of chemical explosions in vacuum, and the resulting loadings on a rigid target.

2. The computational code used is capable of solving time-dependent problems in one space dimension with plane, cylindrical, or spherical symmetry. To effect a compromise between the complex configurations occurring in cases of practical interest and the capabilities of the machine code, the following geometry was decided upon: A spherical charge of high explosive (in this case, pentolite) is detonated at its center, and the detonation products expand outward with spherical symmetry. At a given distance from the origin of coordinates (which is at the center of the charge) is a rigid, spherical wall, concentric with the surface of the spherical charge. The quantities computed are the pressure and energy of the gas as functions of distance and time; and the pressure-time history of the gas at the rigid target.

INITIAL CONDITIONS

3. The computation is begun at the instant the detonation shock reaches the surface of the explosive. It is thus necessary to know the conditions existing in the explosion products at the completion of the detonation process, since these quantities must be used as the initial conditions for the calculation of the expansion. The method used to obtain these initial conditions is that of G. I. Taylor, who solved the problem of determining the mechanical and thermodynamic parameters behind a detonation shock by postulating a similarity solution where all quantities are given as functions of r/t (ref. (a)). It should be noted that the Taylor solution assumes that a spherical detonation wave may be considered to be a stable shock of zero width, proceeding radially outward with constant detonation velocity, and initiating chemical reaction in the material over which it sweeps. Conditions change discontinuously across the shock, and in particular, the substance in front of the shock is completely unreacted, whereas material just behind the shock is completely reacted. Refinements in this detonation concept, such as considerations relating to the existence of a finite reaction zone behind the detonation shock, are not taken into account in this treatment.

4. A machine code that uses the ideas of the Taylor treatment has been written at NOL (ref. (b)), and it is this code that is used to furnish the initial conditions for the calculation of the expansion of the explosion products.

EQUATION OF STATE

5. Many attempts have been made to develop a satisfactory equation of state for the burnt gases behind the detonation shock, ranging from simple perfect gas equations to elaborate solid state equations. It was felt that excessively complex equations of state would not be suitable for the present study, and instead, reliance has been placed on certain results of Deal (ref. (c), (d)) and considerations of Fickett and Wood (ref. (e)) that furnish some evidence to support the belief that, for certain explosives, a constant-gamma, ideal gas law may be used for detonation gas pressures above 500 bars. The gamma for these gases is usually equal to approximately 3. Since, however, we are concerned here with an expansion of the burnt gases into a vacuum, the pressure will certainly fall well below 500 bars, and the equation of state must be extended into this low pressure region.

6. One possibility that immediately suggests itself is simply to let γ be constant over the whole range of pressures encountered in the problem. Another procedure is to take advantage of the fact that at extremely low pressures, gases tend to behave ideally, with a constant value of γ determined only by the molecular structure of the substance. Since the detonation gases will contain, in general, mixtures of diatomic and triatomic gases, the value of γ will be an average, on a molar basis, of various ideal gas gammas. A representative value for the γ of detonation gases at low pressure is $\gamma = 1.35$. The procedure is, then, to construct a function that gives γ as a function of pressure, p , and has the following properties (the particular constants chosen refer to the explosive pentolite):

$$\gamma = 2.682 \text{ (for pentolite)} = \gamma_2 \quad p \geq p_2 = 1000 \text{ bars}$$

$$\gamma = 1.35 = \gamma_1 \quad p \leq p_1 = 100 \text{ bars}$$

$$\frac{d\gamma}{dp} = 0 \quad p = 1000 \text{ bars}$$

$$\frac{d\gamma}{dp} = 0 \quad p = 100 \text{ bars}$$

The curve representing this function has the general appearance of Figure 1.

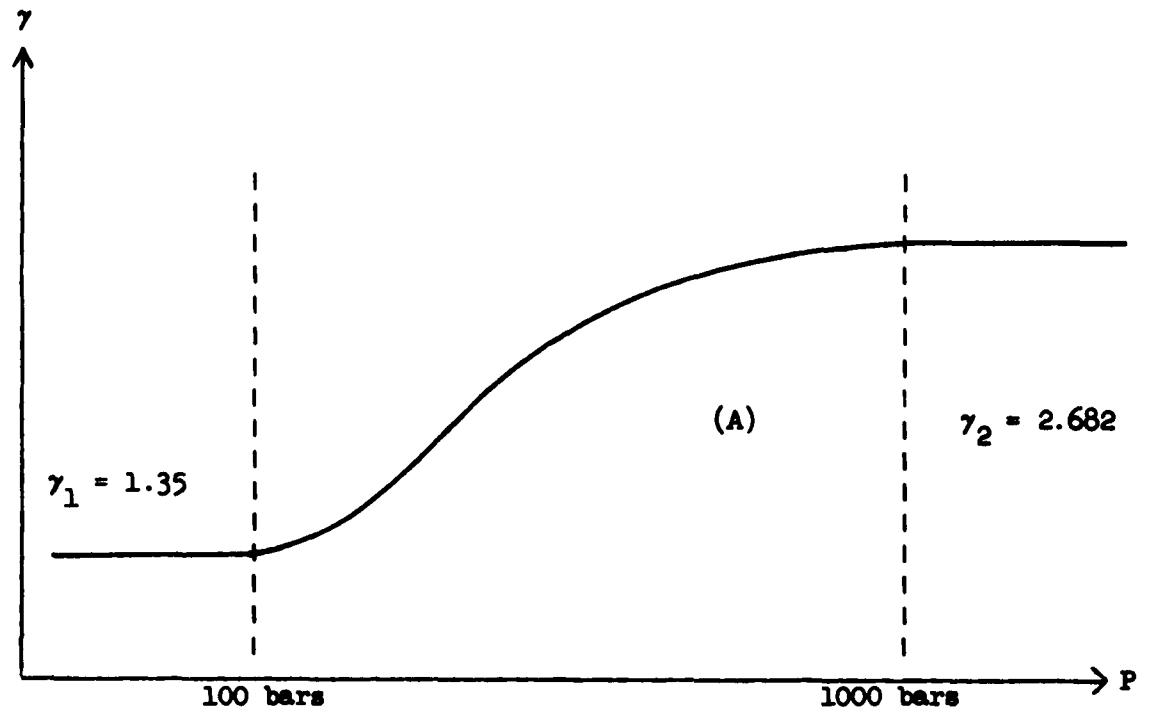


Fig. 1 General Form of γ Versus p Curve

The section (A) of this curve is fitted by a cubic equation:

$$\gamma = A_0 + A_1 p + A_2 p^2 + A_3 p^3 \quad (1)$$

where the constants A_i are given by

$$A_0 = \frac{\gamma_2 p_1 (p_1 - 3p_2) - \gamma_1 p_2^2 (p_2 - 3p_1)}{(p_1 - p_2)^3}$$

$$A_1 = \frac{6p_1 p_2 (\gamma_2 - \gamma_1)}{(p_1 - p_2)^3}$$

$$A_2 = \frac{3(\gamma_1 - \gamma_2) (p_1 + p_2)}{(p_1 - p_2)^3}$$

$$A_3 = \frac{2(\gamma_2 - \gamma_1)}{(p_1 - p_2)^3}$$

7. The functional form (1) for $\gamma = \gamma(p)$ is then used in the ideal gas equation of state $E = \frac{pV}{(\gamma - 1)}$

where E = Energy/gm

p = Pressure

V = Specific volume.

Thus, two schemes have been suggested for construction of the equation of state, one which utilizes a value of γ which is constant over the complete pressure range, and another which fits the interval between a constant high-pressure γ and a constant low-pressure γ by means of a cubic curve giving γ in terms of pressure. Most calculations have been carried out using both forms, so that an indication may be obtained of how sensitive various parameters of interest are to the choice of equation of state.

DESCRIPTION OF THE NUMERICAL COMPUTATION

8. The computations were carried out on an IBM-704 digital computer, using a revised version of the "KO-CODE," a hydrodynamic code originally developed at the Lawrence Radiation Laboratory, Livermore, California (ref. (f)). The prototype difference equations are those of von Neumann and Richtmyer, and the technique used to allow computation beyond shocks is the von Neumann artificial viscosity method (ref. (g), (h)). In this method, a quantity analogous to a viscosity is introduced into the equations for the purpose of smoothing discontinuous shocks so that they extend over a fixed number of spatial zones while maintaining the validity of the Rankine-Hugoniot equations, which relate parameters on both sides of the shock. Consequently, the machine program does not find it necessary to deal with discontinuous changes in the calculated quantities, and any shocks that appear in the problem are properly propagated, although with some rounding of the normally steep shock front.

9. The calculation is carried out by dividing the spherical region into a given number of spatial zones, not necessarily all of the same radial length. At each interface a mass particle is localized and a given particle will always remain at the same interface. Each mass particle has associated with it a velocity, so that velocities are calculated at the interfaces; quantities like pressure, specific volume, and total energy density are localized in the regions between interfaces, that is, at the centers of spatial zones.

10. When the expanding gases reach the spherical wall, the velocity of the boundary is set equal to zero, and the kinetic energy thus lost is added to the last spatial zone as internal energy, thus raising the pressure in this last zone. The pressure continues to rise as the gases move toward the wall, and a compression shock moves inward toward the origin.

11. The NOL computing facility includes equipment for the display on a cathode ray tube screen of various quantities as they are computed. Photographs of such plots are presented in this report, and include distributions of pressure and energy density with distance at various times.

RESULTS

12. Before numerical data are presented, a brief qualitative description of the results will be given. Upon the completion of the detonation process, the explosion gas expands into the vacuum, with a consequent drop in pressure at the gas boundary and an increase in the velocity of the boundary. The pressure at the gas-vacuum interface quickly drops to an essentially zero value, and the boundary acquires a constant radial velocity. As the gas expands, the kinetic energy in the system increases, at the expense of the internal energy. When the gas boundary strikes the wall, a compression shock is formed that proceeds inward toward the origin. At any given time, the pressure between the shock and the wall appears to be fairly constant, though this constant level decreases with time. As the shock proceeds inward, most of the kinetic energy of the gas is converted back into internal energy. When the reflected shock reaches the origin, it is reflected back into the gas as another compression shock. These shocks are reflected back and forth between the wall and the origin until some sort of stable equilibrium is reached. Since the entire process takes place within a fixed, constant volume, it is expected that the final equilibrium state is one of stationary gas, with energy, pressure, and volume related by the ideal gas law having the appropriate value of γ . However, the computations reported upon here do not go far enough in time to demonstrate this final equilibrium.

13. The calculations made refer to a one-pound sphere of pentolite, density = 1.65 gm/cc, detonated at its center, for various values of wall distance. Pressure and energy density curves are given in Figures 8-11, plotted against radial distance from the origin.

14. Each point represents the value of the quantity being considered at a point half-way between the positions of adjacent mass points, and always remains associated with the same two mass points. Thus, the plots present not only a pressure (or energy) versus distance picture, but also indicate the motion of the mass particles in time. The energy quantity plotted is an energy per unit volume, multiplied by $4\pi r^2$, where r is the radial distance from the origin. Thus, the area under the curve between

any two radial distance values is equal to the energy contained in the corresponding portion of the system. The interchange between internal and kinetic energy thus becomes clearly visible from the plots.

15. One can see from the pressure plots the rounding of the shock front and the pressure oscillations immediately behind the shock front; these are characteristics peculiar to the particular computational method used, namely the von Neumann-Richtmyer "q" method.

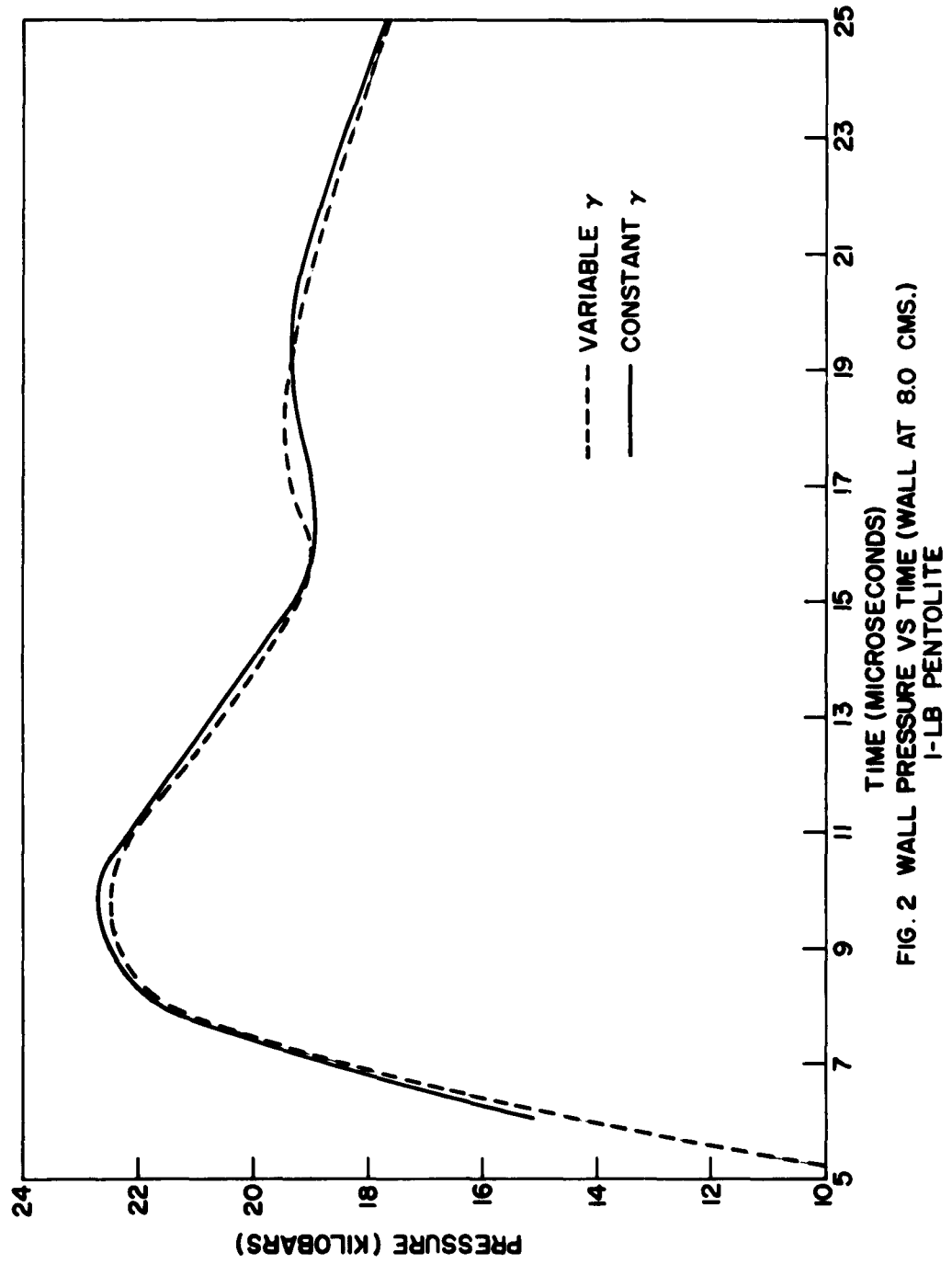
16. In the tables, numerical results are given for various wall distances from the origin. The quantities listed are time, in microseconds, with the zero of the time scale being taken as the instant in which the detonation shock reaches the outer surface of the explosive charge; the kinetic energy, internal energy, and total energy (in megabars-cm³) present in the system at a given time; and the shock position (in centimeters) and wall pressure (in bars), as functions of time. Due to the finite difference method of calculation, the total energy is not exactly conserved, as it should be in a precise computation. The range of variation of the total energy can be seen to be small relative to the magnitude of the energy transferred between the kinetic and internal modes. Table 1 and Table 2 both refer to a wall at 8.0 centimeters, but the calculations given in Table 2 use the alternative variable γ equation of state. Tables 3, 4, and 5 refer to walls at the distances 16.0 cms., 24.0 cms., and 32.85 cms., respectively, and each represents a tabulation using the constant gamma equation of state. Figures 2-6 present plots of the wall pressure versus time for various wall distances, using both forms of the equation of state. For small wall distances, where the pressure at the wall remains well above 1000 bars, the two calculations give fairly identical results. However, for intermediate distances, when the wall pressure lies in the 100-1000 bar range, the results begin to diverge, and for large wall distances, with pressures well below 100 bars, the variable γ equation of state gives substantially lower pressures. This behavior can be seen most clearly from Figure 7, which gives the peak wall pressure versus distance, for both equations of state. The true equation of state probably yields curves which lie between these two extremes.

SCALING

17. The only characteristic length that appears in this problem is the initial charge radius, and therefore all lengths may be expressed in terms of this quantity. Furthermore, the initial distribution of mechanical and thermodynamic parameters (that is, the Taylor Wave) depends only on the properties of the solid explosive and is self-similar with respect to the charge radius. Consequently, the results given in this report for specific distances, times, and explosive weights also apply to situations in which times and distances are multiplied by a factor k , and the explosive weight is multiplied by k^3 . For example, it can be seen from Figure 7 that for one pound of pentolite, a peak pressure of 10 bars (145 psi) is obtained at the wall when the wall is approximately 100 cms. from the origin. Thus, a 512-pound pentolite charge ($k=8$) will generate a pressure of 145 psi at a wall located approximately 800 cms. or 26 feet, from the center of the charge. Such a pressure is believed to be high enough to destroy a spacecraft.

CONCLUDING REMARKS

18. The results presented here constitute a preliminary investigation of the loading of structures by explosions in rarefied atmospheres. The next step is to run calculations with air of varying densities in the space between the explosive and wall, and to study the air or blast effect. It would also be extremely interesting to substitute for an idealized rigid target, a substance that may be compressed, or that may be pushed as a result of the explosion. Another goal for the future is the use of more practical geometries, perhaps with the use of 2-dimensional machine codes, and more sophisticated equations of state for the detonation gases, such as that of Kistiakowsky and Wilson.



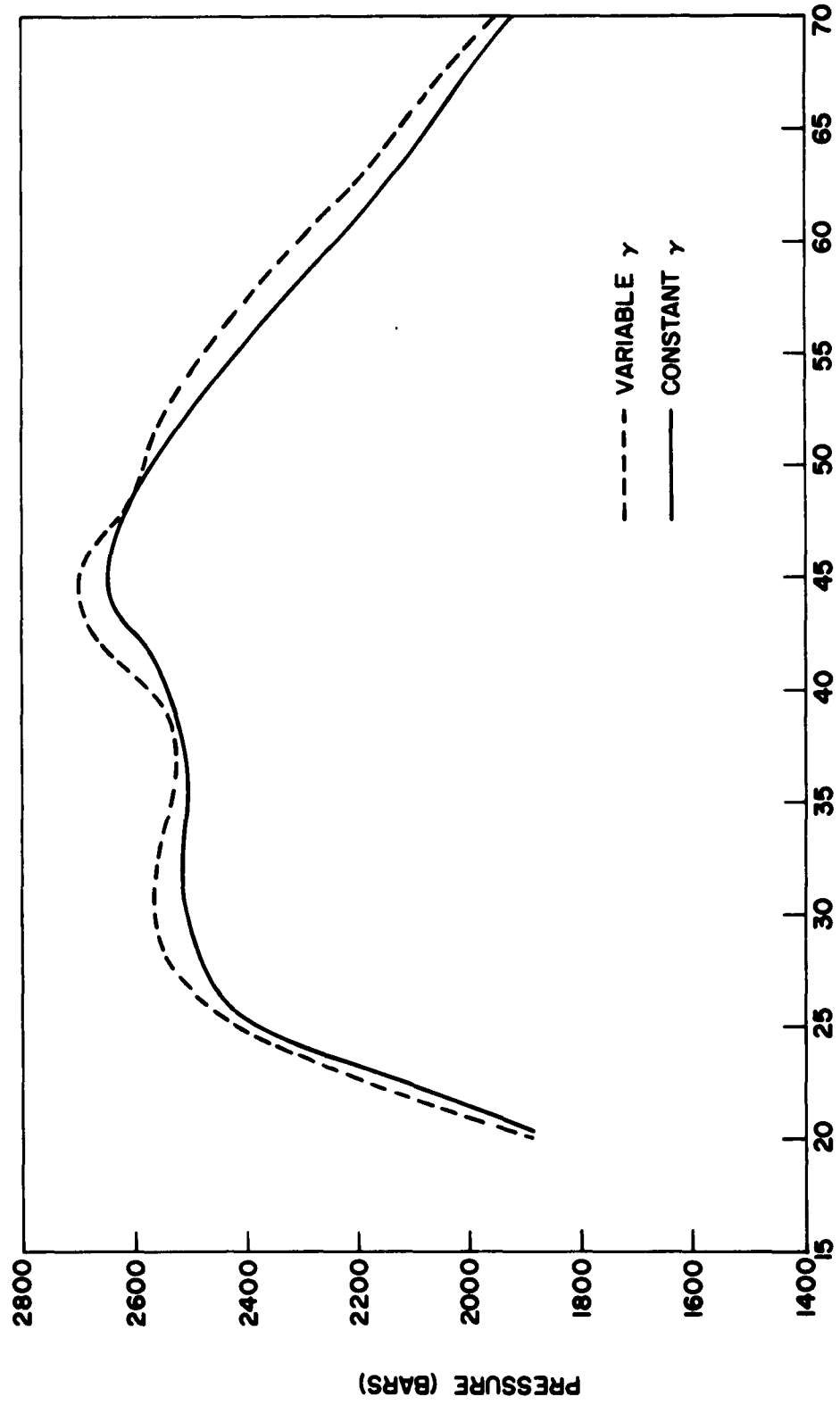


FIG. 3 WALL PRESSURE VS TIME (WALL AT 16.0 CMS.)
1-LB PENTOLITE

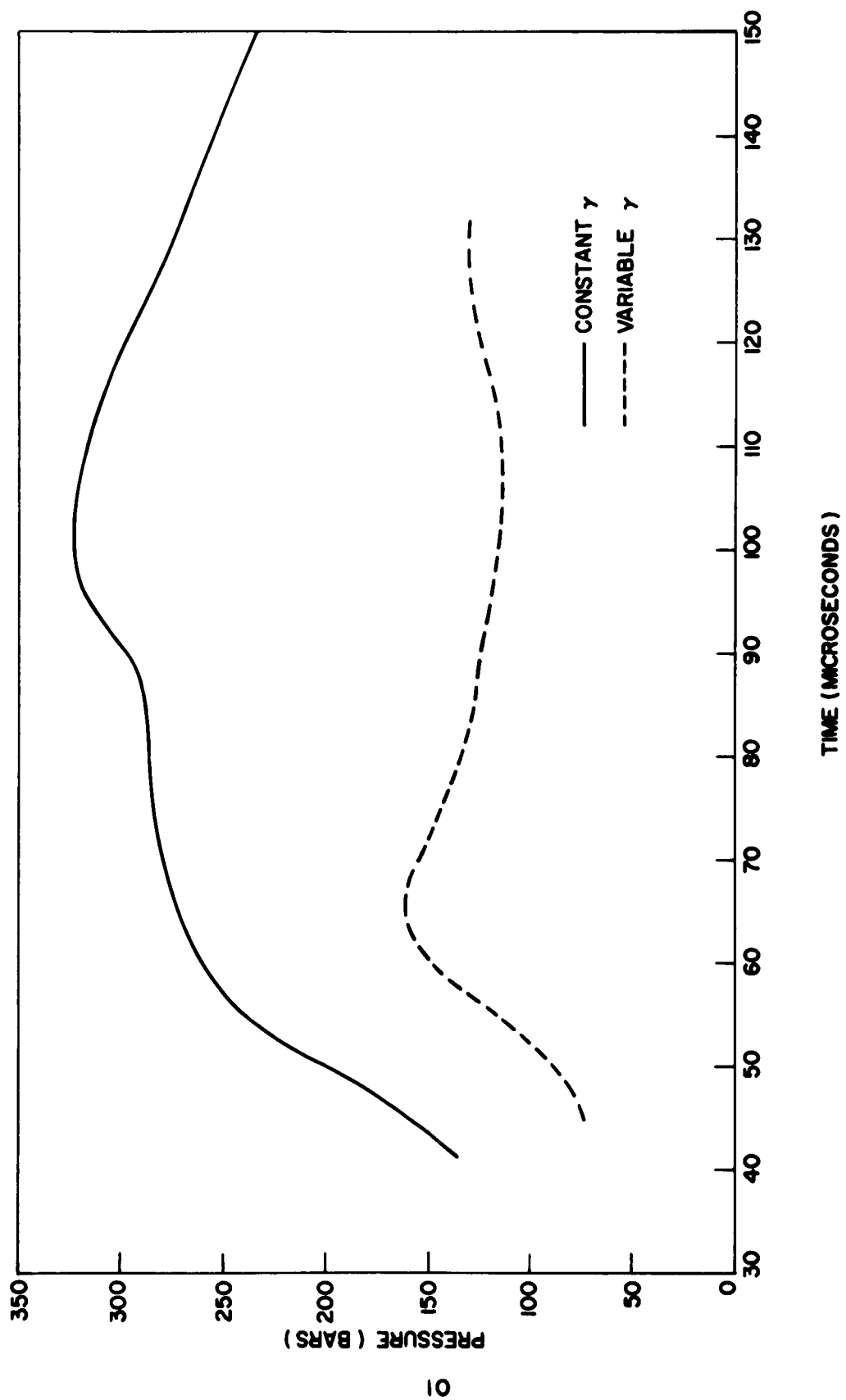


FIG. 4 WALL PRESSURE VS TIME (WALL AT 32.8 CMS.)
1-LB PENTOLITE

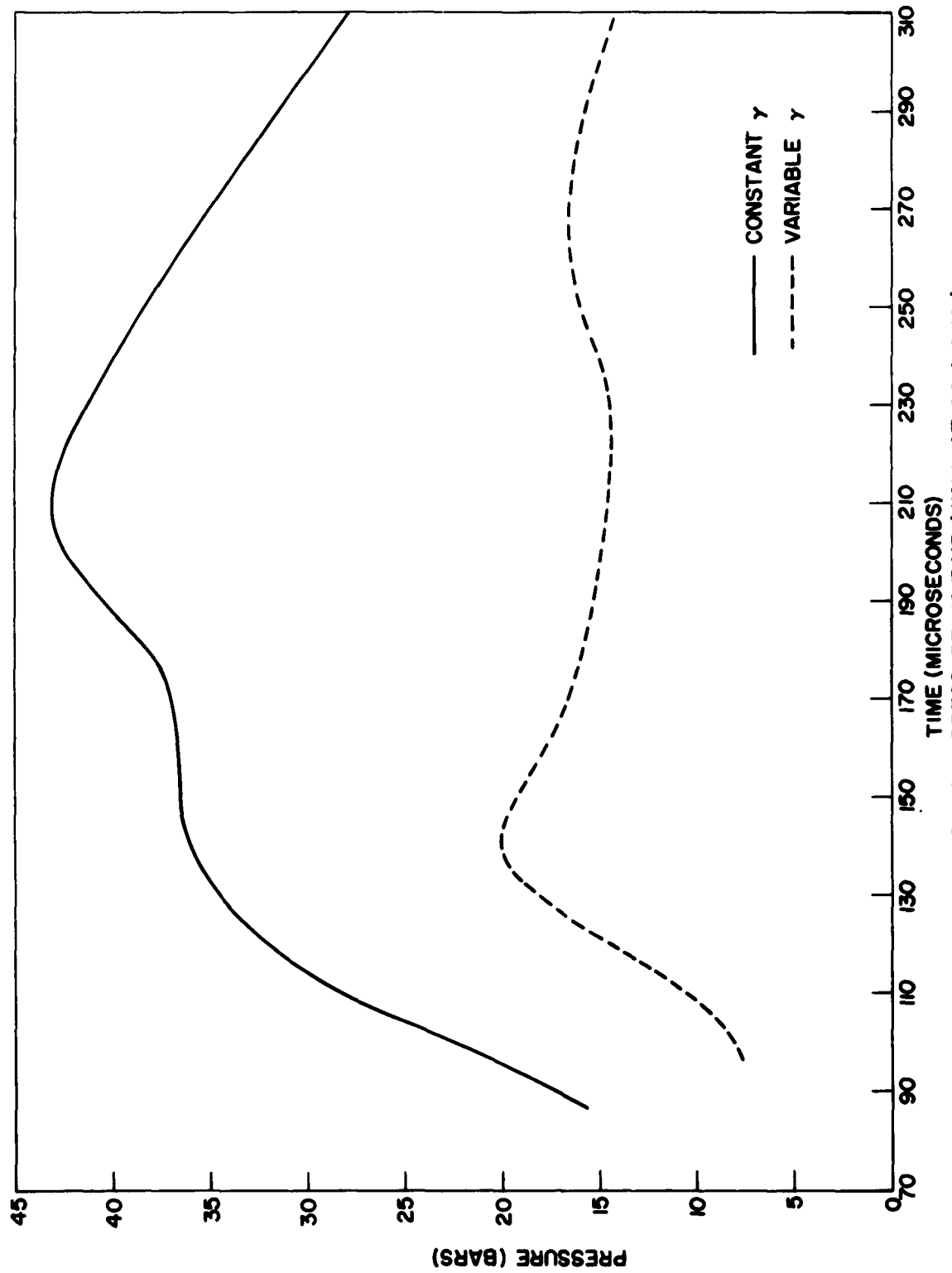


FIG. 5 WALL PRESSURE VS TIME (WALL AT 64.4 CMS.)
 1-LB PENTOLITE

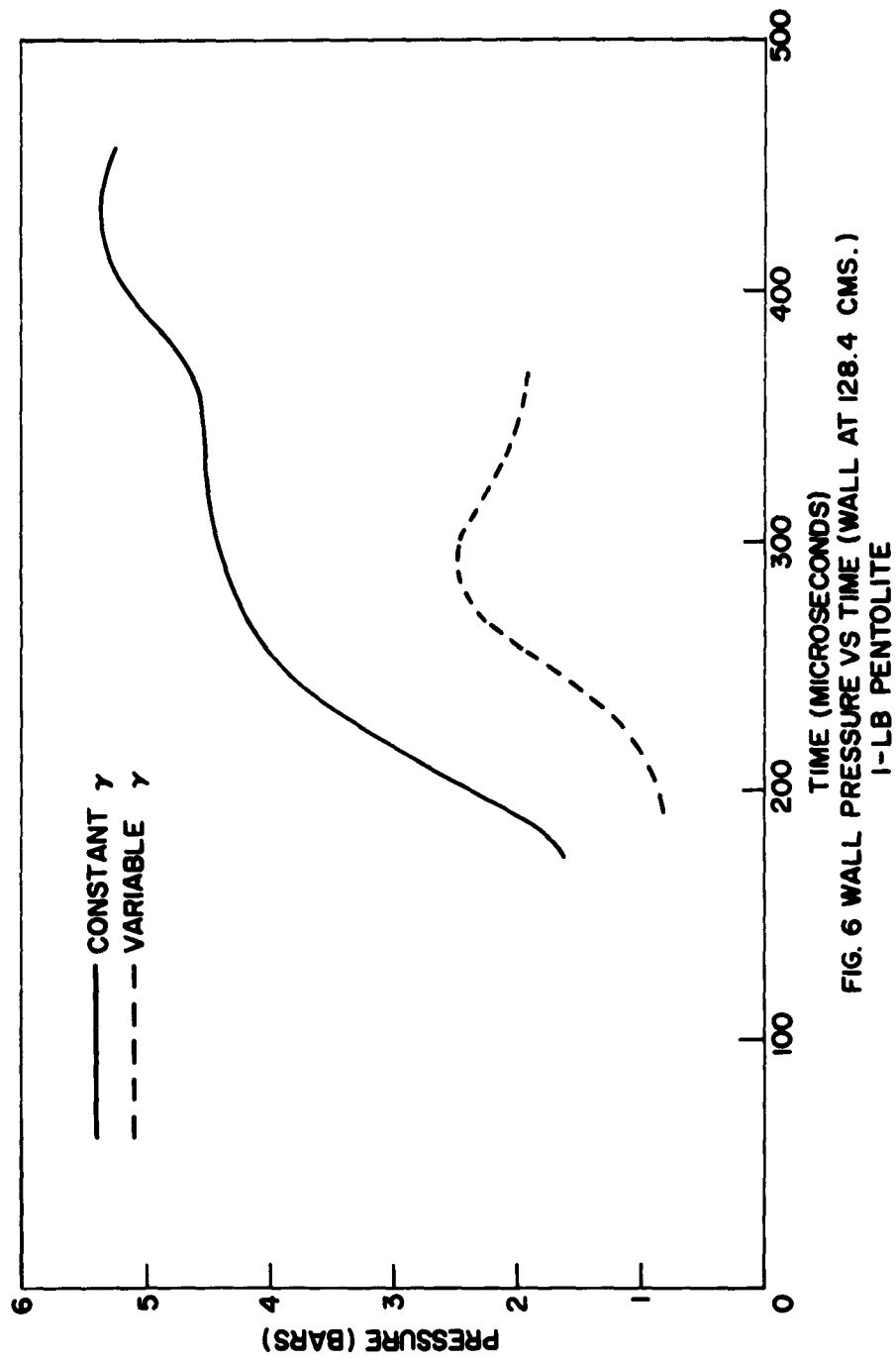


FIG. 6 WALL PRESSURE VS TIME (WALL AT 128.4 CMS.)
1-LB PENTOLITE

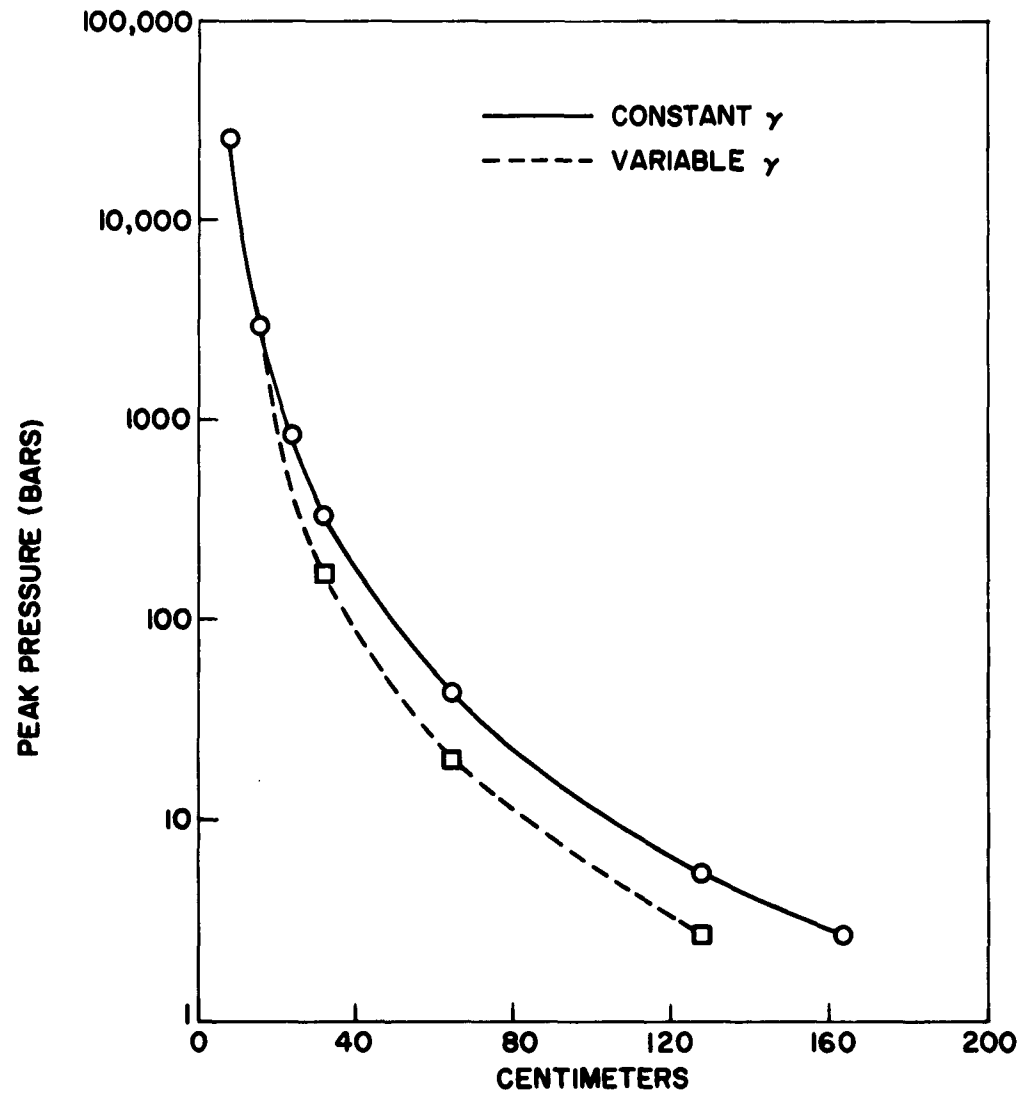


FIG. 7 PEAK PRESSURE VS WALL DISTANCE
1-LB PENTOLITE

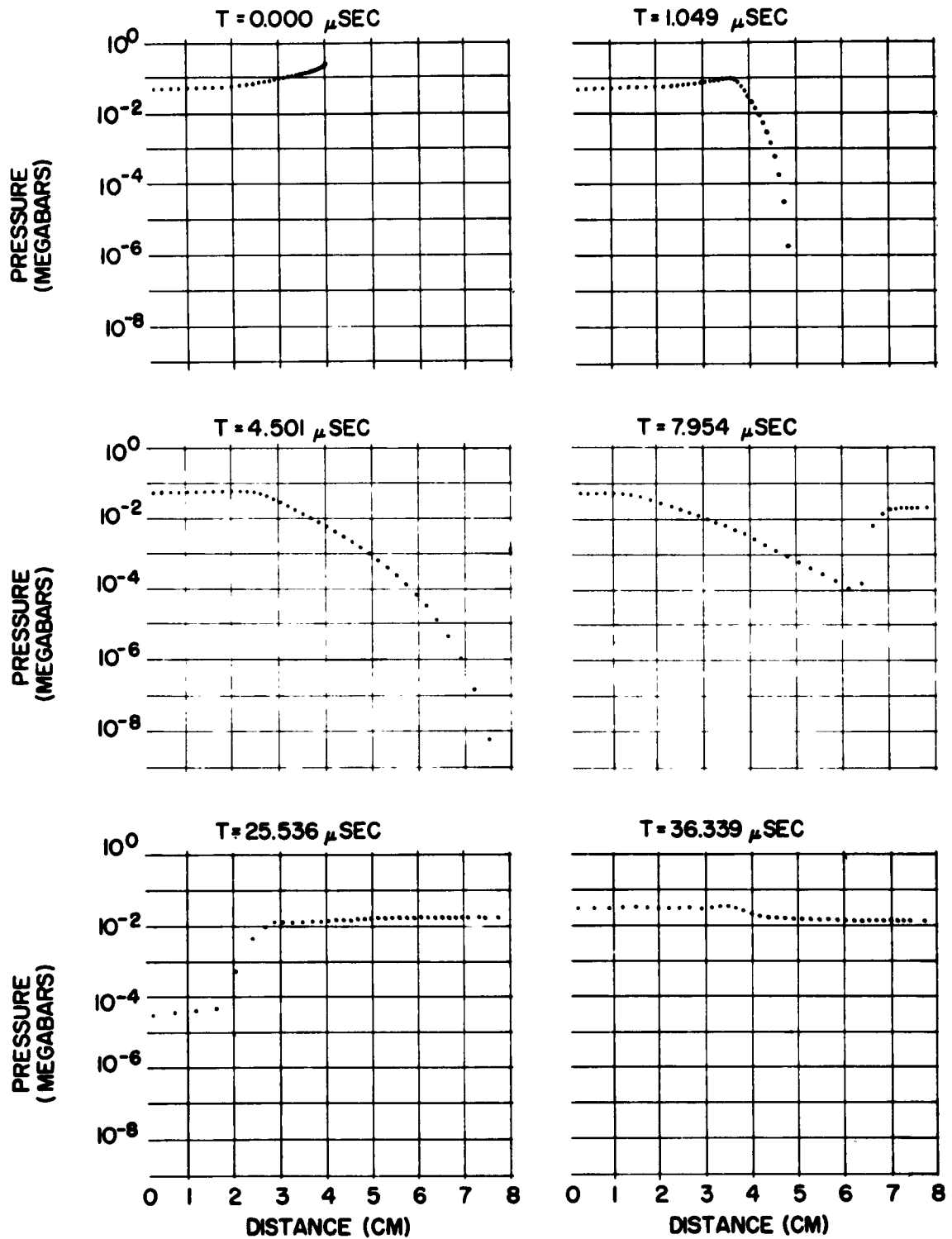


FIG 8 PRESSURE (MEGABARS) VS DISTANCE, WALL AT 8.0 CM, GAMMA = 2.682. 1-LB PENTOLITE

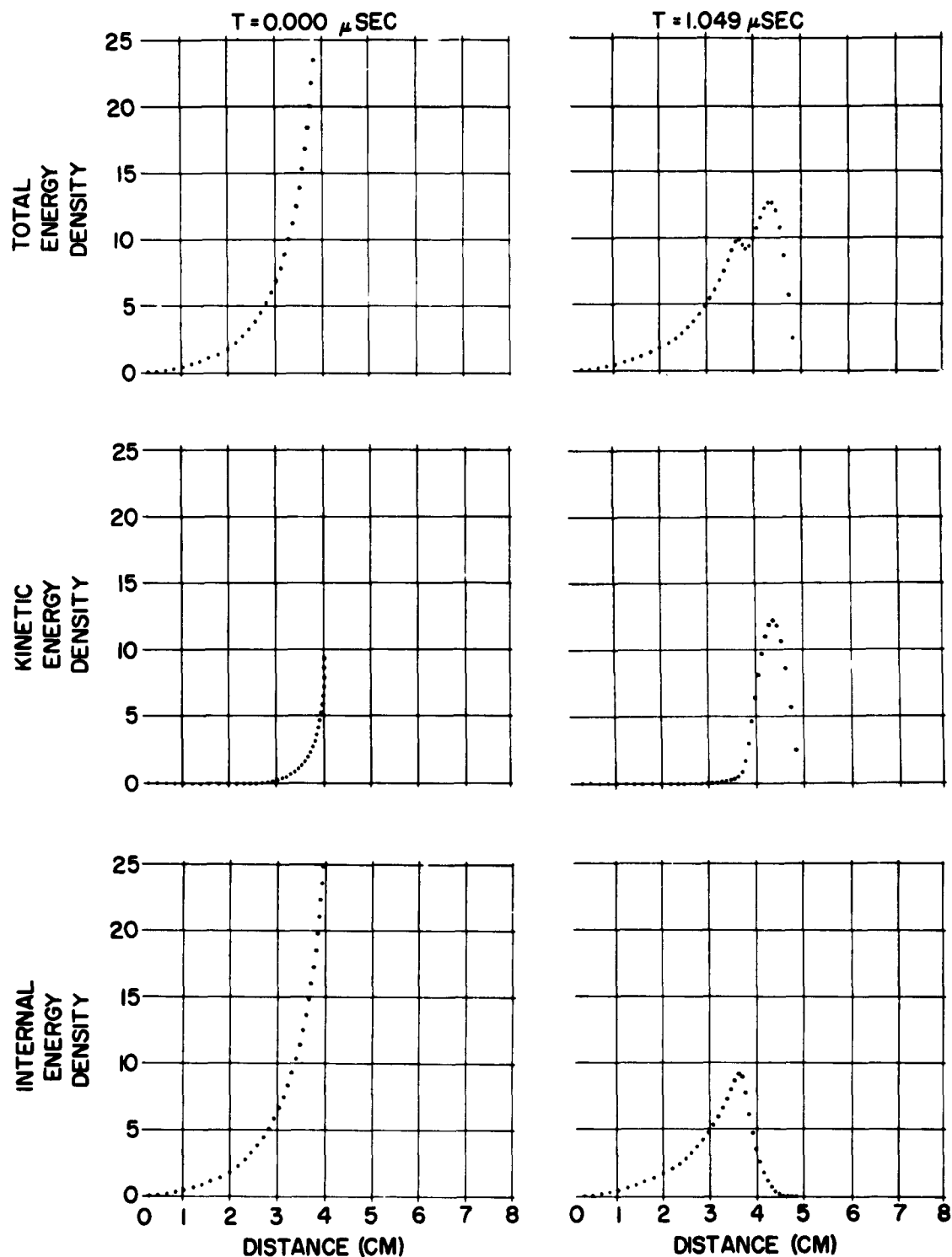


FIG. 9 ENERGY DENSITY (ENERGY / VOLUME $\times 4 \pi R^2$, IN UNITS OF MEGABAR - CM^2). WALL AT 8.0 CM, GAMMA = 2.682. AREA UNDER CURVE EQUALS ENERGY IN UNITS OF MEGABAR - CM^3 1-LB PENTOLITE

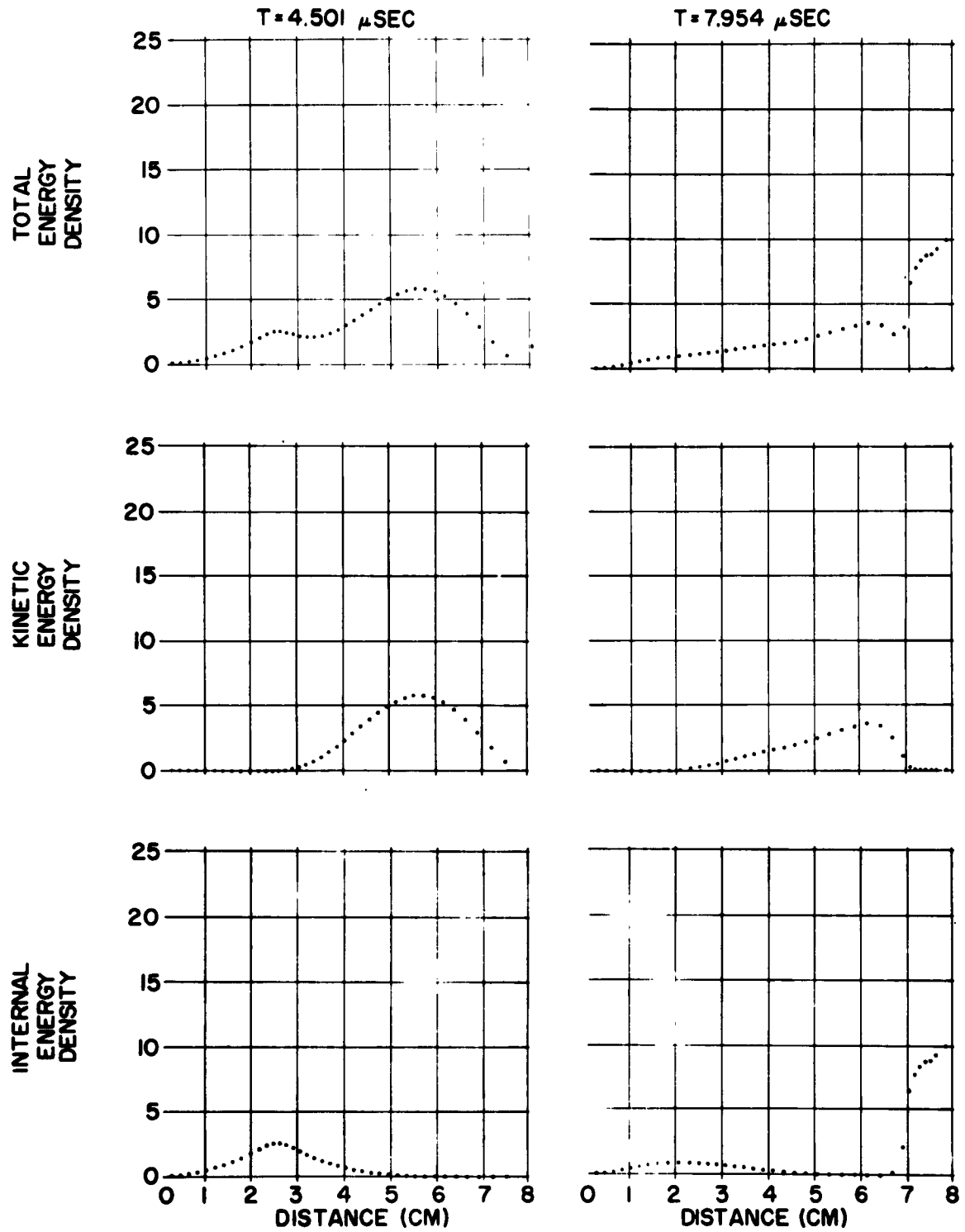


FIG. 10 ENERGY DENSITY (ENERGY / VOLUME $\times 4\pi R^2$, IN UNITS OF MEGABAR - CM^2). WALL AT 8.0 CM, GAMMA = 2.682. AREA UNDER CURVE EQUALS ENERGY IN UNITS OF MEGABAR - CM^3 . 1-LB PENTOLITE

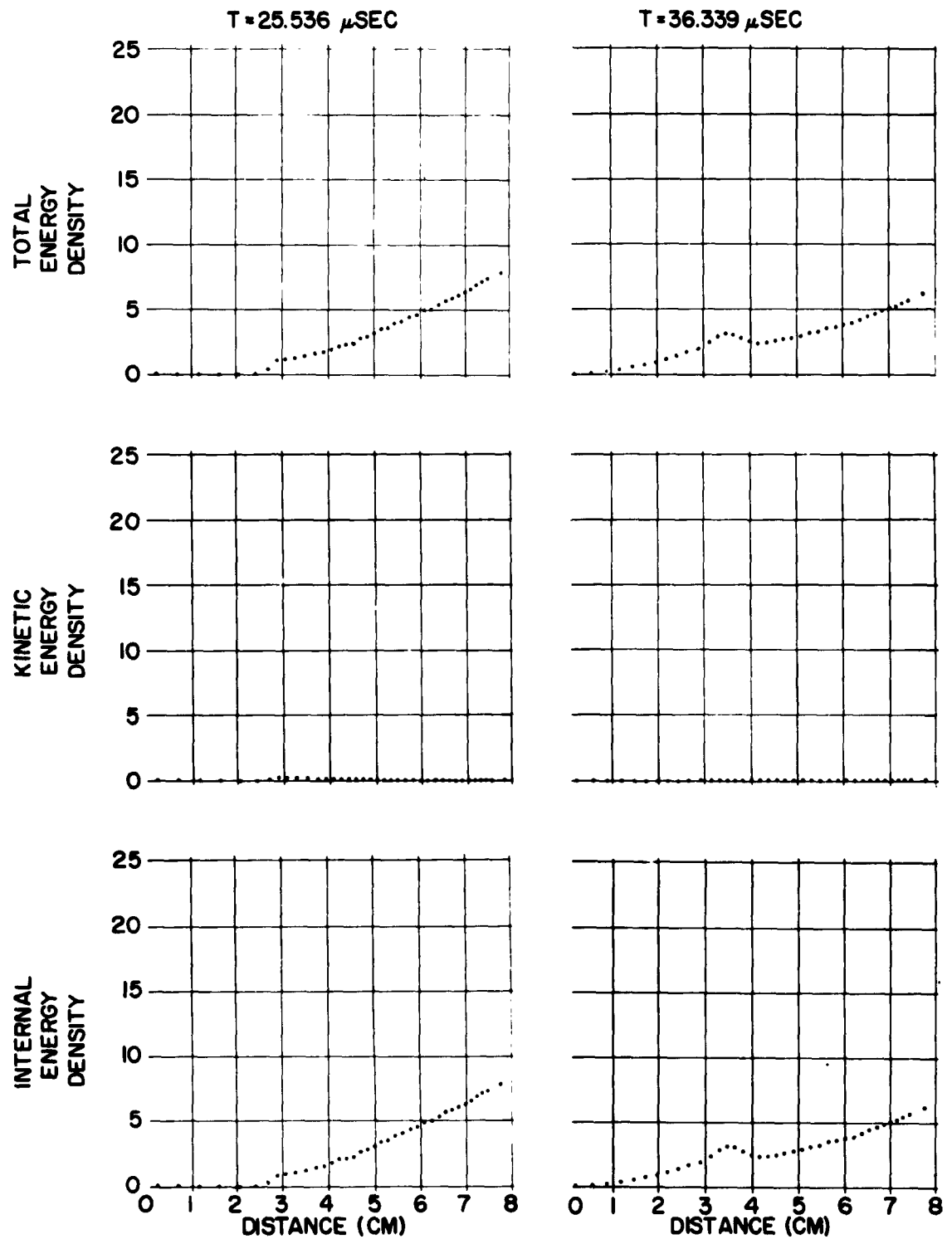


FIG. 11 ENERGY DENSITY (ENERGY / VOLUME $\times 4\pi R^2$, IN UNITS OF MEGABAR- CM^2). WALL AT 8.0 CM, GAMMA = 2.682. AREA UNDER CURVE EQUALS ENERGY IN UNITS OF MEGABAR- CM^3 . 1-LB PENTOLITE

Table 1

WALL AT 8.0 CENTIMETERS; $\gamma = 2.682$
ONE POUND PENTOLITE

Time (μ secs)	Kinetic Energy ← (Megabars-Cm ³)	Internal Energy	Total Energy →	Shock Position (Cms)	Wall Pressure (Bars)
4.939 (Wall Struck)					
5.019	15.745	5.231	20.976	7.559	3753.9
6.840	11.587	9.602	21.189	7.037	18212.0
7.954	9.178	12.007	21.185	6.890	21628.1
8.951	7.438	13.752	21.190	6.662	22603.8
10.028	6.004	15.181	21.185	6.400	22712.4
11.008	5.033	16.147	21.180	6.087	22096.0
12.031	4.242	16.934	21.176	5.961	21401.0
13.016	3.578	17.597	21.175	5.630	20648.7
14.016	2.925	18.249	21.174	5.325	19934.7
15.031	2.306	18.866	21.172	5.220	19310.1
17.019	1.338	19.829	21.167	4.804	19062.1
18.542	0.825	20.338	21.163	4.332	19300.8
20.022	0.487	20.674	21.161	3.994	19348.7
21.037	0.339	20.819	21.158	3.768	19074.0
22.010	0.277	20.879	21.156	3.512	18736.3
22.518	0.271	20.884	21.155	3.511	18642.8
23.025	0.280	20.874	21.154	3.261	18421.5
24.041	0.330	20.823	21.153	3.002	18092.6
25.018	0.407	20.745	21.152	2.723	17797.6
27.042	0.619	20.532	21.151	2.031	16920.9
28.021	0.715	20.436	21.151	1.616	16660.4
29.268	0.787	20.366	21.153	0.733	16336.5
30.250	0.732	20.422	21.154	0.191	16028.6
First Shock Reaches Center					
31.015	0.589	20.568	21.157	1.374	15582.0
32.286	0.449	20.709	21.158	1.885	15066.6
33.264	0.323	20.835	21.158	2.565	14469.3
34.271	0.232	20.925	21.157	2.826	14264.4
35.196	0.178	20.979	21.157	3.270	14126.7
39.169	0.226	20.927	21.153	4.869	13308.3
41.687	0.461	20.690	21.151	6.018	13272.5
44.213	0.662	20.491	21.153	7.757	15711.1

Reflected Shock Reaches Wall

Table 1 (Cont'd)

Time (μ secs)	Kinetic Energy ← (Megabars-Cm ³) →	Internal Energy	Total Energy	Shock Position (Cms)	Wall Pressure (Bars)
46.701	0.400	20.756	21.156	6.479	19734.3
49.192	0.183	20.971	21.154	5.571	19701.0
51.683	0.119	21.035	21.154	4.816	18890.0
54.174	0.148	21.005	21.153	3.977	17887.8
56.712	0.237	20.915	21.152	3.247	17052.1
59.203	0.368	20.785	21.153	2.179	16369.2
Reflected Shock Reaches Center					
61.693	0.416	20.738	21.154	1.078	15830.9
64.171	0.178	20.978	21.156	1.674	15266.4
66.715	0.093	21.061	21.154	2.916	14912.2
69.206	0.131	21.022	21.153	4.110	14606.4
71.698	0.217	20.936	21.153	4.995	14387.0
74.190	0.314	20.840	21.154	6.099	14488.3
76.681	0.358	20.798	21.156	7.766	17132.0

Table 2

WALL AT 8.0 CENTIMETERS; Variable γ
ONE POUND PENTOLITE

Time (μ secs)	Kinetic Energy ← (Megabars-Cm ³)	Internal Energy →	Total Energy	Shock Position (Cms)	Wall Pressure (Bars)
4.984 (Wall Struck)					
5.514	14.747	6.499	21.246	7.486	11333.3
6.507	12.473	8.775	21.249	7.152	16231.1
7.993	9.187	12.053	21.240	6.902	21629.6
8.989	7.470	13.776	21.246	6.669	22385.9
10.015	6.085	15.156	21.241	6.406	22476.4
11.006	5.085	16.152	21.237	6.096	22131.2
15.026	2.336	18.892	21.228	5.230	19301.1
16.014	1.805	19.420	21.225	4.933	19006.3
16.443	1.603	19.621	21.224	4.877	19168.2
19.021	0.705	20.513	21.218	4.356	19431.3
22.028	0.279	20.932	21.211	3.512	18704.2
25.036	0.414	20.792	21.206	2.716	17746.6
25.380	0.448	20.759	21.207	2.696	17521.3

Table 3

WALL AT 16.0 CENTIMETERS; $\gamma = 2.682$
ONE POUND PENTOLITE

Time (μ secs)	Kinetic Energy ← (Megabars-Cm ³)	Internal Energy →	Total Energy	Shock Position (Cms)	Wall Pressure (Bars)
14.892	(Expanding Gases Strike Wall)				
16.243	19.042	2.277	21.319	14.499	1075.8
21.223	13.817	7.508	21.325	13.290	1966.5
26.262	9.104	12.214	21.318	12.397	2447.3
33.757	4.653	16.653	21.306	11.197	2506.8
43.745	1.091	20.201	21.292	9.660	2644.4
50.727	0.315	20.971	21.286	8.231	2561.4
55.737	0.481	20.800	21.281	7.230	2395.4
60.729	0.950	20.328	21.278	5.435	2212.7
65.733	1.428	19.852	21.280	3.601	2056.1
68.198	1.546	19.737	21.282	1.638	1976.1
Reflected Shock Reaches Center					
73.305	1.041	20.251	21.292	3.980	1763.9
78.209	0.468	20.824	21.292	6.141	1663.2
83.239	0.210	21.077	21.287	8.208	1555.4
88.270	0.442	20.840	21.282	10.085	1507.0
93.300	0.959	20.323	21.282	12.4912	1485.7
98.214	1.270	20.022	21.292	15.453	2259.3
Reflected Shock Reaches Wall					
100.785	1.063	20.229	21.292	13.138	2434.2
105.763	0.645	20.646	21.291	11.432	2507.5
110.755	0.323	20.967	21.290	10.279	2450.2
115.747	0.155	21.133	21.288	9.087	2399.5
120.739	0.200	21.087	21.286	7.760	2336.4
125.731	0.445	20.840	21.285	5.752	2231.6

Table 4

WALL AT 24.0 CENTIMETERS; $\gamma = 2.682$
ONE POUND PENTOLITE

Time (μ secs)	Kinetic Energy ← (Megabars-Cm ³)	Internal Energy →	Total Energy	Shock Position (Cms)	Wall Pressure (Bars)
24.848	(Expanding Gases Strike Wall)				
27.859	18.861	2.455	21.316	21.785	285.4
29.085	18.114	3.241	21.355	21.201	379.4
34.150	14.668	6.685	21.353	20.158	515.6
39.122	11.468	9.880	21.348	19.005	636.7
41.630	10.051	11.297	21.348	18.748	673.5
46.601	7.687	13.655	21.342	18.081	714.1
51.598	5.819	15.516	21.335	16.734	726.6
61.372	2.760	18.581	21.341	15.601	731.0
66.430	1.630	19.706	21.336	14.826	773.4
71.378	0.867	20.465	21.332	14.334	805.6
76.381	0.428	20.900	21.328	13.194	794.9
81.383	0.301	21.022	21.323	12.643	765.7
91.377	0.775	20.541	21.316	9.560	693.9
101.487	1.567	19.749	21.316	5.835	618.4
106.433	1.810	19.511	21.321	2.623	579.6
108.864	1.800	19.522	21.322	0.777	561.2
Reflected Shock Reaches Center					
111.403	1.584	19.743	21.327	2.713	535.2
113.922	1.330	20.003	21.333	5.335	517.8
115.741	1.142	20.192	21.334	6.740	501.3

Table 5

WALL AT 32.849 CENTIMETERS; $\gamma = 2.682$
ONE POUND PENTOLITE

Time (μ secs)	Kinetic Energy ← (Megabars-Cm ³) →	Internal Energy	Total Energy	Shock Position (Cms)	Wall Pressure (Bars)
35.795	(Expanding Gases Strike Wall)				
41.547	18.153	3.297	21.450	28.662	139.076
46.509	15.823	5.628	21.451	27.710	174.486
51.551	13.453	7.995	21.448	26.824	215.729
56.484	11.291	10.152	21.443	25.801	245.894
61.455	9.377	12.065	21.442	24.655	265.639
66.503	7.728	13.707	21.435	24.461	275.381
71.551	6.339	15.090	21.429	23.266	279.206
76.599	5.085	16.342	21.427	22.362	280.554
86.557	2.822	18.597	21.419	21.257	285.344
91.567	1.946	19.470	21.416	20.673	298.743
96.590	1.257	20.156	21.413	20.002	314.907
101.524	0.763	20.647	21.410	19.197	318.806
106.580	0.440	20.966	21.406	18.165	316.141
111.574	0.297	21.106	21.403	17.466	308.708
116.569	0.326	21.073	21.399	16.549	299.212
121.563	0.487	20.910	21.397	15.537	288.742
129.107	0.894	20.501	21.395	13.232	271.972
141.446	1.660	19.734	21.394	8.151	243.706
146.455	1.890	19.507	21.397	5.856	232.512
148.986	1.953	19.446	21.399	3.608	225.779
151.403	1.956	19.445	21.401	1.143	220.213

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